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Access DB# <u>\$5098</u>

SEARCH REQUEST FORM

Scientific and Technical Information Center

| Requester's Full Name: S. Art Unit: 1681 Phone I Mail Box and Bldg/Room Location | Number 30 <u>& ५</u> 5% | Serial Number: | 14 Date: 1/24/03 10/03/48/ cle): PAPER DISK E-MAIL | |
|---|--|---|---|---|
| If more than one search is subm | itted, please prioriti | ze searches in order of | need. ME | |
| Please provide a detailed statement of the Include the elected species or structures, I utility of the invention. Define any terms known. Please attach a copy of the cover | search topic, and describe teywords, synonyms, acros that may have a special m | as specifically as possible the nyms, and registry numbers, a eaning. Give examples or rele | nd combine with the concept or | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |
| Title of Invention: | \cup 1 | inum sait frech | neons and their use on produ | H |
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| *For Sequence Searches Only* Please include appropriate serial number. A | de all pertinent information (| | ed patent numbers) along with the Jan Delaval Reference Librarian Biotechnology & Chemical Library CM1 1E07 – 703-308-4498 jan delaval@uspto.gov | |
| Zis Ge Car x is bond | | b optionally r (a) | wended/hy c. ska. | |
| See claim) for 19/50 Fee claims | 8, 10, 12 | 14, + 15. | · · · · · · · · · · · · · · · · · · · | |
| C) cym 12. | H-Rb | Rois Room | T, Tis -2/2 | C.V. |
| Re is Ry or U | 1, 11 is 5 | 4-4. R3 | 2 | |
| STAFF USE ONLY Searcher: | Type of Search NA Sequence (#) | Vendors and cost | ************************************** | |
| Searcher Phone #: 4498 | AA Sequence (#) | Dialog | | |
| Searcher Location: | Structure (#) | Questel/Orbit | 2.0 100 | |
| Date Searcher Picked Up: 2/3/3 | Bíbliographic | Dr.Link | 90 表 图 | ľ |
| Date Completed: | Litigation | Lexis/Nexis | 9 5 10 | |
| learcher Prep & Review Time: | Fulltext | Sequence Systems | | |
| Slerical Prep Time: | Patent Family | WWW/Internet | | |
| Inline Time: + Us | Other | Other (specify) | | |
| TO-1590 (8-01) | | | # | |

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Mary Hale, Supervisor, 308-4258 CM-1 Room 1E01

| Voluntary Results Feedback Fo |
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| > I am an examiner in Workgroup: (Example: 1610) |
|--|
| > Relevant prior art found, search results used as follows: |
| 102 rejection |
| 103 rejection |
| Cited as being of interest. |
| Helped examiner better understand the invention. |
| Helped examiner better understand the state of the art in their technology. |
| Types of relevant prior art found: |
| Foreign Patent(s) |
| Non-Patent Literature (journal articles, conference proceedings, new product announcements etc.) |
| > Relevant prior art not found: |
| Results verified the lack of relevant prior art (helped determine patentability). |
| Search results were not useful in determining patentability or understanding the invention. |
| Other Comments: |
| ullet |
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FILE COVERS 1907 - 3 Feb 2003 VOL 138 ISS 6 FILE LAST UPDATED: 2 Feb 2003 (20030202/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS
L50
     2001:63952 HCAPLUS
ΑN
    134:131521
DN
    Preparation of neutral prodrugs of bisquaternaryammonium
ΤI
    parasiticides
    Vial, Henri; Calas, Michele; Ancelin,
IN
    Marie-Laure; Bourguignon, Jean-Jacques; Vidal,
    Valerie; Rubi, Eric
    Centre National de la Recherche Scientifique (C.N.R.S.), Fr.
PΑ
SO
    PCT Int. Appl., 85 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    French
TC
    ICM C07C211-09
         CO7C327-30; CO7C323-27; CO7C323-59; CO7D277-22; CO7D277-24;
         C07D277-30; C07D295-14; A61K031-14; A61K031-145; A61K031-425;
         A61P033-06; C07D327-06
    28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
    Section cross-reference(s): 1
FAN.CNT 1
                     KIND DATE
                                          APPLICATION NO.
                                                          DATE
    PATENT NO.
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                                          _____
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    WO 2001005742
                    A1 20010125
                                         WO 2000-FR2122 20000721 <--
PΤ
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
            HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
            LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
            SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
            YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
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     FR 2796642
                     A1
                           20010126
                                         FR 1999-9471
                                                           19990721 <--
    FR 2796642
                           20011019
                      В1
                         20020417
                                         EP 2000-958598
                                                         20000721 <--
    EP 1196371
                     A1
           AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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BR 2000012601
                            20020521
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PRAI FR 1999-9471
                      Α
                            19990721
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                      W
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     WO 2000-FR2122
os:
     MARPAT 134:131521
     Title compds., e.g., Z[N(CHO)CR2:GR3SRa]2 [I; Ra = R, SR,COR; R =
AΒ
     (un) substituted alkyl, -Ph, heterocyclylmethyl, etc.; R2 = H, alkyl,
     alkoxycarbonylmethyl; R3 = H, alk(en)yl, etc.; RR3,R2R3 = atoms to
     complete a ring; Z = (heteroatom- or arylene-interrupted)(satd.) alkylene]
     were prepd. Thus, 5-(2-hydroxymethyl)-4-methylthiazole was condensed with
     Br(CH2)12Br to give the bisthiazolium dibromide (drug) which was
     biscondensed with PrSSO3Na (prepn. given) to give I [Ra = SPr, R2 = Me, R3
     = CH2CH2OH, Z = (CH2)12](prodrug). Data for biol. activity of title
     compds. were given.
     prodrug bisquaternaryammonium parasiticide;
ST
     antimalarial bisquaternaryammonium prodrug
IT
     Antimalarials
       Parasiticides
        (prepn. of neutral prodrugs of bisquaternaryammonium
       parasiticides)
IT
     321915-72-4P 321915-73-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); MFM (Metabolic formation); RCT (Reactant); SPN
     (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
     FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or
     reagent); USES (Uses)
        (prepn. of neutral prodrugs of bisquaternaryammonium
       parasiticides)
TΤ
     321915-74-6P 321915-75-7P 321915-76-8P
     321915-77-9P 321915-78-0P 321915-79-1P
     321915-80-4P 321915-81-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (prepn. of neutral prodrugs of bisquaternaryammonium
       parasiticides)
     321915-50-8P 321915-51-9P 321915-52-0P
     321915-53-1P 321915-54-2P 321915-55-3P
     321915-56-4P 321915-57-5P 321915-58-6P
     321915-59-7P 321915-60-0P 321915-61-1P
     321915-62-2P 321915-63-3P 321915-64-4P
     321915-65-5P 321915-66-6P 321915-67-7P
     321915-68-8P 321915-69-9P 321915-70-2P
     321915-71-3P 321915-82-6P 321915-83-7P
     321915-84-8P 321915-85-9P 321915-92-8P
     321915-93-9P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of neutral prodrugs of bisquaternaryammonium
        parasiticides)
ΙT
     98-88-4, Benzoyl chloride
                                 100-07-2, p-Methoxybenzoyl chloride
                                106-94-5, Propyl bromide 108-29-2,
     100-39-0, Benzyl bromide
                            109-89-7, Diethylamine, reactions
                                                                 110-91-8,
     .gamma.-Valerolactone
                           137-00-8, 4-Methyl-5-(2-hydroxyethyl)thiazole
     Morpholine, reactions
     141-97-9, Ethyl acetoacetate 629-09-4, 1,6-Diiodohexane
                                                                693-95-8,
                        1642-81-5, 4-Chloromethylbenzoic acid
                                                                3003-84-7,
     4-Methylthiazole
                                   3344-70-5, 1,12-Dibromododecane
     Tetrahydrofurfuryl chloride
                                                                     5259-98-3,
                           7377-26-6, Benzoic acid, 4-chlorocarbonyl, methyl
     5-Chloro-1-pentanol
             7735-42-4, Hexadecane-1,16-diol
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of neutral prodrugs of bisquaternaryammonium
        parasiticides)
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т*т 2751-70-4P 6313-36-6P 6363-00-4P 24772-65-4P, 1,12-Diiodododecane 24772-67-6P, 1,16-Diiodohexadecane 51023-75-7P 62642-59-5P 62642-62-0P 89585-19-3P 98316-89-3P, 77339-73-2P 4-Methyl-5-(2-methoxyethyl)thiazole 106261-54-5P 123742-32-5P 321915-88-2P **321915-89-3P** 321915-86-0P 321915-87-1P 321915-91-7P 321915-90-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of neutral prodrugs of bisquaternaryammonium parasiticides) RE.CNT THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD RE (1) Hikoichi, H; US 3278537 A 1966 (2) Libman, D; JOURNAL OF THE CHEMICAL SOCIETY 1952, P2305 HCAPLUS (3) Lopez-Calahorra, F; HETEROCYCLES 1994, V37(3), P1570 (4) Marti; TETRAHEDRON LETT 1993, V34(3), P521 HCAPLUS (5) Mitchell, R; CHEMICAL ABSTRACTS 1961, V55(12) (6) Mitchell, R; J PHARMACOL EXPTL THERAP 1961, V131, P334 HCAPLUS (7) Virbac Sa; FR 2751967 A 1998 HCAPLUS (8) Zirkle, C; US 3131220 A 1964 HCAPLUS 321915-72-4P 321915-73-5P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of neutral prodrugs of bisquaternaryammonium parasiticides) RN321915-72-4 HCAPLUS Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-hydroxyethyl)-4-methyl-, CN dibromide (9CI) (CA INDEX NAME)

●2 Br-

RN 321915-73-5 HCAPLUS
CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-methoxyethyl)-4-methyl-, dibromide (9CI) (CA INDEX NAME)

●2 Br-

TT 321915-74-6P 321915-75-7P 321915-76-8P 321915-77-9P 321915-78-0P 321915-79-1P 321915-80-4P 321915-81-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of neutral prodrugs of **bisquaternaryammonium** parasiticides)

RN 321915-74-6 HCAPLUS

CN Thiazolium, 3,3'-(1,12-dodecanediyl)bis[4-methyl-, diiodide (9CI) (CA INDEX NAME)

2 I-

RN 321915-75-7 HCAPLUS

CN Thiazolium, 3,3'-(1,16-hexadecanediyl)bis[5-(2-methoxyethyl)-4-methyl-, diiodide (9CI) (CA INDEX NAME)

●2 I-

PAGE 1-A

PAGE 2-A

I-

RN

321915-77-9 HCAPLUS
Thiazolium, 5,5'-[1,6-hexanediylbis(oxy-2,1-ethanediyl)]bis[4-methyl-3-(phenylmethyl)-, dibromide (9CI) (CA INDEX NAME) CN

PAGE 1-A

PAGE 2-A

RN 321915-78-0 HCAPLUS

CN Thiazolium, 5,5'-(1,12-dodecanediyl)bis[4-(2-ethoxy-2-oxoethyl)-3-methyl-, diiodide (9CI') (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O} \\ & \text{N}^+ & \text{CH}_2 - \text{C} - \text{OEt} \\ & \text{S} & & \\ & \text{(CH}_2) 12 \\ & \text{EtO} - \text{C} - \text{CH}_2 \\ & \text{O} & & +_{\text{N}} & \\ & & \text{Me} \end{array}$$

●2 I-

RN 321915-79-1 HCAPLUS

CN Thiazolium, 5,5'-(1,12-dodecanediyl)bis[4-(2-ethoxy-2-oxoethyl)-3-(phenylmethyl)-, dibromide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-Ph & O \\ & & | \\ N^+ & CH_2-C-OEt \\ & & \\ (CH_2) 12 \\ \\ EtO-C-CH_2 & \\ & & \\ O & +N \\ \end{array}$$

●2 Br-

RN 321915-80-4 HCAPLUS

CN Thiazolium, 4,4'-(1,12-dodecanediyl)bis[3-methyl-, diiodide (9CI) (CA INDEX NAME)

●2 T-

RN 321915-81-5 HCAPLUS

CN Thiazolium, 4,4'-(1,12-dodecanediyl)bis[3-(phenylmethyl)-, dibromide (9CI) (CA INDEX NAME)

●2 Br-

IT 321915-50-8P 321915-51-9P 321915-52-0P 321915-53-1P 321915-54-2P 321915-55-3P 321915-56-4P 321915-57-5P 321915-58-6P 321915-59-7P 321915-60-0P 321915-61-1P 321915-62-2P 321915-63-3P 321915-64-4P 321915-65-5P 321915-66-6P 321915-67-7P 321915-68-8P 321915-69-9P 321915-70-2P 321915-71-3P 321915-82-6P 321915-83-7P 321915-84-8P 321915-85-9P 321915-92-8P 321915-93-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of neutral prodrugs of bisquaternaryammonium parasiticides)

RN 321915-50-8 HCAPLUS

CN Formamide, N, N'-1, 12-dodecanediylbis[N-[4-hydroxy-1-methyl-2-[[(tetrahydro-2-furanyl)methyl]dithio]-1-butenyl]- (9CI) (CA INDEX NAME)

RN 321915-51-9 HCAPLUS

CN Formamide, N,N'-1,12-dodecanediylbis[N-[4-hydroxy-1-methyl-2-(propyldithio)-1-butenyl]- (9CI) (CA INDEX NAME)

RN 321915-52-0 HCAPLUS

CN Formamide, N, N'-1, 12-dodecanediylbis[N-[4-hydroxy-1-methyl-2-[(phenylmethyl)dithio]-1-butenyl]- (9CI) (CA INDEX NAME)

RN 321915-53-1 HCAPLUS

CN Formamide, N, N'-1, 12-dodecanediylbis[N-[4-hydroxy-2-[(2-hydroxyethyl)dithio]-1-methyl-1-butenyl]- (9CI) (CA INDEX NAME)

RN 321915-54-2 HCAPLUS

CN Formamide, N, N'-1, 12-dodecanediylbis[N-[4-methoxy-1-methyl-2-(propyldithio)-1-butenyl]- (9CI) (CA INDEX NAME)

RN 321915-55-3 HCAPLUS

CN Formamide, N, N'-1, 12-dodecanediylbis[N-[1-methyl-2-(propyldithio)ethenyl]-(9CI) (CA INDEX NAME)

RN 321915-56-4 HCAPLUS

CN Ethanethioic acid, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

RN 321915-57-5 HCAPLUS

CN Propanethioic acid, 2,2-dimethyl-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

RN 321915-58-6 HCAPLUS

CN Benzenecarbothioic acid, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

RN 321915-59-7 HCAPLUS

CN Benzenecarbothioic acid, 4-methoxy-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

RN 321915-60-0 HCAPLUS

CN Benzenecarbothioic acid, 4-[2-(4-morpholinyl)ethoxy]-, S,S'-[1,12-dodecanediylbis((formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

- CH $_2-$ OMe

RN 321915-61-1 HCAPLUS

CN Benzenecarbothioic acid, 4-[(diethylamino)methyl]-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 321915-62-2 HCAPLUS

CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

PAGE 1-B

RN 321915-63-3 HCAPLUS

CN Benzoic acid, 4,4'-[5,18-diformyl-3,20-bis(2-methoxyethyl)-4,19-dimethyl-1,22-dioxo-2,21-dithia-5,18-diazadocosa-3,19-diene-1,22-diyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)

RN 321915-64-4 HCAPLUS

CN Benzenecarbothioic acid, S,S'-[1,16-hexadecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

RN 321915-65-5 HCAPLUS

CN Formamide, N, N'-1, 12-dodecanediylbis[N-[1-(2-oxo-1, 3-oxathian-4-ylidene)ethyl]- (9CI) (CA INDEX NAME)

RN 321915-66-6 HCAPLUS

CN Benzenecarbothioic acid, 4-methoxy-, S,S'-[1,6-hexanediylbis[oxy[1-[1-(formylmethylamino)ethylidene]-3,1-propanediyl]]] ester (9CI) (CA INDEX NAME)

PAGE 1-B

RN 321915-67-7 HCAPLUS

CN Benzenecarbothioic acid, 4-methoxy-, S,S'-[1,6-hexanediylbis[oxy[1-[1-[formyl(phenylmethyl)amino]ethylidene]-3,1-propanediyl]]] ester (9CI) (CA INDEX NAME)

PAGE 1-B

RN 321915-68-8 HCAPLUS

CN 3,17-Eicosadienedioic acid, 4,17-bis(benzoylthio)-3,18-bis(formylmethylamino)-, diethyl ester (9CI) (CA INDEX NAME)

RN 321915-69-9 HCAPLUS

CN 3,17-Eicosadienedioic acid, 4,17-bis(benzoylthio)-3,18-bis[formyl(phenylmethyl)amino]-, diethyl ester (9CI) (CA INDEX NAME)

RN 321915-70-2 HCAPLUS

CN Benzenecarbothioic acid, S,S'-[2,15-bis(formylmethylamino)-1,15-hexadecadiene-1,16-diyl] ester (9CI) (CA INDEX NAME)

RN 321915-71-3 HCAPLUS

CN Benzenecarbothioic acid, S,S'-[2,15-bis[formyl(phenylmethyl)amino]-1,15-hexadecadiene-1,16-diyl] ester (9CI) (CA INDEX NAME)

RN 321915-82-6 HCAPLUS

CN 1,16-Hexadecanediamine, N,N'-bis(5-chloropentyl)-N,N'-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 321915-83-7 HCAPLUS

CN 1,16-Hexadecanediamine, N,N'-bis(4-chloropentyl)-N,N'-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 321915-84-8 HCAPLUS

CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, ethanedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 321915-62-2

CMF C50 H74 N4 O8 S2

PAGE 1-A

PAGE 1-B

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 321915-85-9 HCAPLUS

CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, (2R,3R)-2,3-dihydroxybutanedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 321915-62-2 CMF C50 H74 N4 O8 S2

PAGE 1-A

PAGE 1-B

CM · 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 321915-92-8 HCAPLUS

CN Formamide, N, N'-1, 12-dodecanediylbis[N-[2-[[2-(diethylamino)ethyl]dithio]-4-methoxy-1-methyl-1-butenyl]- (9CI) (CA INDEX NAME)

RN 321915-93-9 HCAPLUS

CN Formamide, N, N'-1, 12-dodecanediylbis[N-[4-(benzoyloxy)-1-methyl-2-(propyldithio)-1-butenyl]- (9CI) (CA INDEX NAME)

IT 321915-86-0P 321915-89-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of neutral prodrugs of bisquaternaryammonium

parasiticides)

RN 321915-86-0 HCAPLUS

CN Thiazole, 5,5'-[1,6-hexanediylbis(oxy-2,1-ethanediyl)]bis[4-methyl- (9CI) (CA INDEX NAME)

RN 321915-89-3 HCAPLUS

CN 4-Thiazoleacetic acid, 5,5'-(1,12-dodecanediyl)bis-, diethyl ester (9CI) (CA INDEX NAME)

=> =>

=> d 151 bib abs tot

L51 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2003 ACS

AN 2002:426419 HCAPLUS

DN 138:32620

TI New drugs against malaria with special reference to effectors of plasmodial phospholipid metabolism

AU Vial, Henri J.; Vidal-Sailhant, Valerie; Ancelin, Marie L.; Herbute, Serge; Martin, Dominique; Baunaure, F.; Calas, Michele

CS UMR 5539 CNRS, Montpellier, 34095, Fr.

Multi-Drug Resistance in Emerging and Re-Emerging Diseases, [Joint Symposium on Multiple Drug Resistance and Emerging Diseases], New Delhi, India, Feb. 28-Mar. 4, 1999 (2000), Meeting Date 1999, 175-189. Editor(s): Mahajan, R. C.; Therwath, Amu. Publisher: Indian National Science Academy, New Delhi, India. CODEN: 69CQYH; ISBN: 81-7319-346-0

DT Conference; General Review

LA English

A review. The increasing multidrug resistance of malarial AB parasites to conventional antimalarial agents makes very acute the need for novel drugs, since, today, none of them can offer protection against malaria in all regions of the world. Drug development efforts generally aim for compds. that work through new, independent mechanisms of action and that are structurally unrelated to existing antimalarial agents. From this perspective, thorough biol. and biochem. studies of the parasite could lead to the discovery of a specific target that could be used in the design of original compds. capable of exterminating the parasite without injuring the host. Phospholipid biosynthesis in Plasmodium is of crucial importance considering the high degree of membrane biogenesis. Phospholipid metab. developed by Plasmodium during its intraerythrocytic cycle is essential and constitutes a novel pharmacol. target. The most promising interference is the blockade of the choline transporter protein, which provides Plasmodium with a precursor for the synthesis of phosphatidylcholine, the major phospholipid of infected erythrocytes. The 1st 2 generations of active lead compds. consisted of quaternary ammonium salts and amidine compds. The most prominent characteristics of these new mols. are: potent in vitro antimalarial activity against resistant P. falciparum strains and isolates, similar in vitro and in vivo activity against P.

vivax, absence of in vitro resistance induction under long-term drug pressure, in vivo activity in various murine species and P. falciparum-infected Aotus monkeys even at very high parasitemia, lack of recurrence, and absence of genotoxicity. Although tolerance was improved with the 2nd generation of compds., their intestinal absorption remained low. An original strategy has been initiated to design neutral prodrugs which require biotransformation once in the serum compartment (i.e., after passing through the intestinal barrier) to confer antimalarial activity. These prodrugs showed the same high in-vitro antimalarial activity (nM), tolerance (i.p. LD50 increased by 100-250-fold compared to cationic drugs) and high relative absorption (improved by 10-15-fold compared to cationic drugs). The antimalarial activity of these compds. is very satisfactory; all these considerations mean that the approach is now quite realistic. Overall, this pharmacol. approach is novel and should allow the design of candidates for initiating preclin. studies.

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L51 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2003 ACS
- AN 2000:60210 HCAPLUS
- DN 132:231503
- TI Antimalarial Activity of Compounds Interfering with Plasmodium falciparum Phospholipid Metabolism:

 Comparison between Mono- and Bisquaternary Ammonium Salts
- AU Calas, Michele; Ancelin, Marie L.; Cordina, Gerard; Portefaix, Philippe; Piquet, Gilles; Vidal-Sailhan, Valerie; Vial, Henri
- CS Laboratoire des Aminoacides Peptides et Proteines, CNRS UMR 5810 Universite de Montpellier II, Montpellier, 34095, Fr.
- SO Journal of Medicinal Chemistry (2000), 43(3), 505-516 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- LA English
- On the basis of a previous structure-activity relationship study, we AB identified some essential parameters, e.g. electronegativity and lipophilicity, required for polar head analogs to inhibit Plasmodium falciparum phospholipid metab., leading to parasite death. To improve the in vitro antimalarial activity, 36 cationic choline analogs consisting of mono-, bis-, and triquaternary ammonium salts with distinct substituents of increasing lipophilicity were synthesized. For monoquaternary ammonium salts, an increase in the lipophilicity around nitrogen was beneficial for antimalarial activity: IC50 decreased by 1 order of magnitude from tri-Me to tri-Pr substituents. Irresp. of the polar head substitution (Me, Et, hydroxyethyl, pyrrolidinium), increasing the alkyl chain length from 6 to 12 methylene groups always led to increased The highest activity was obtained for the N,N,N-tripropyl-Ndodecyl substitution of nitrogen (IC50 33 nM). Beyond 12 methylene groups, the antimalarial activities of the compds. decreased The structural requirements for bisquaternary ammonium salts in antimalarial activity were very similar to . those of monoquaternary ammonium salts, i.e. polar head steric hindrance and lipophilicity around nitrogen (Me, hydroxyethyl, Et, pyrrolidinium, etc.). In contrast, with bisquaternary ammonium salts, increasing the lipophilicity of the alkyl chain between the two nitrogen atoms (from 5 to 21 methylene groups) constantly and dramatically increased the activity. Most of these duplicated mols. had activity around 1 nM, and the most lipophilic compd. synthesized exhibited an IC50 as low as 3 pM (21 methylene groups). Globally, this oriented synthesis produced 28 compds. out of 36 with an IC50 lower than 1 .mu.M, and 9 of them had an IC50 in the nanomolar range, with 1 compd. in the picomolar

range. This indicates that developing a pharmacol. model for antimalarial compds. through choline analogs is a promising strategý.

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 24 ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L51 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2003 ACS
- 1998:105729 HCAPLUS
- DN. . . 128:: 238968
- Antimalarial activity of 77 phospholipid polar head analogs: close correlation between inhibition of phospholipid metabolism and in vitro Plasmodium falciparum growth
- Ancelin, Marie L.; Calas, Michele; Bompart, Jacques; ΑU Cordina, Gerard; Martin, Dominique; Bari, Mohammed Ben; Jei, Taib; Druilhe, Pierre; Vial, Henri J.
- CNRS UMR 5539, Department of Biologie-Sante, Montpellier, 34095, Fr. CS
- Blood (1998), 91(4), 1426-1437 SO CODEN: BLOOAW; ISSN: 0006-4971
- PB W. B. Saunders Co.
- Journal DT
- English LA
- AB Seventy-seven potential analogs of phospholipid polar heads, choline and ethanolamine, were evaluated in vitro as inhibitors of Plasmodium falciparum growth. Their IC50 ranged from 10-3 to 10-7 mol/L. Ten compds. showed similar antimalarial activity when tested against three different parasite strains (2 chloroquinesensitive strains and 1 chloroquine-resistant strain). Compds. showing marked antimalarial activity were assayed for their effects on phospholipid metab. The most active compds. (IC50 of 1 to 0.03 .mu.mol/L) were inhibitors of de novo phosphatidylcholine (PC) biosynthesis from choline. For a series of 50 compds., there was a close correlation between impairment of phospholipid biosynthesis and inhibition of in vitro malaria parasite growth. High choline concns. caused a marked specific shift in the curves for PC biosynthesis inhibition. Concns. inhibiting 50% PC metab. from choline were in close agreement with the Ki of these compds. for the choline transporter in Plasmodium knowlesi-infected erythrocytes. By contrast, measurement of the effects of 12 of these compds. on rapidly dividing lymphoblastoid cells showed a total absence of correlation between parasite growth inhibition and human lymphoblastoid cell growth inhibition. Specific antimalarial effects of choline or ethanolamine analogs are thus likely mediated by their alteration of phospholipid metab. This indicates that de novo PC biosynthesis from choline is a very realistic target for new malaria chemotherapy, even against pharmacoresistant strains.
- L51 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2003 ACS
- 1998:98316 HCAPLUS
- DN
- Preparation of .alpha.,.omega.-bis(quaternary ammonium)alkane ΤI salt antimalarial and antibabesiasis agents
- Vial, Henri; Calas, Michele; Ancelin,
- Marie-Laure; Giral, Louis
- Virbac S.A., Fr.; Vial, Henri; Calas, Michele; Ancelin, Marie-Laure; PA Giral, Louis ,
- SO PCT Int. Appl., 50 pp. CODEN: PIXXD2
- DT Patent
- LA French
- FAN.CNT 1

PΙ

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| | | | | |
| WO 9804252 | A1 | 19980205 | WO 1997-FR1336 | 19970717 |

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kumar - 10 / 031486
        W: BR, CA, CN, JP, KR, US
         RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
                            19980206
                                           FR 1996-9678
                                                             19960731
     FR 2751967
                       Α1
                            19981009
     FR 2751967
                       В1
                                           EP 1997-934589
                                                             19970717
     EP 917465
                       A1
                            19990526
     EP 917465
                            20021120
                       В1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, FI
                            19990817
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                                                             19970717
     BR 9710629
                       Α
                                           CN 1997-197753
                                                             19970717
     CN 1232388
                       Α
                            19991020
                       T2
                            20001128
                                           JP 1998-508541
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     JP 2000515877
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                                           AT 1997-934589
                                                             19970717
     AT 227984
                                                             19990201
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     US 6096788
                                           KR 1999-700769
                                                             19990929
     KR 2000029690
                       Α
                            20000525
PRAI FR 1996-9678
                       Α
                            19960731
     WO 1997-FR1336
                       W
                            19970717
OS
     MARPAT 128:127745
     The title compds. R1(R2)(R3)N+XN+(R3)(R2)R1 [I; R1 = C1-20 hydrocarbyl;
AΒ
     R2, R3 = (un) substituted C1-20 hydrocarbyl; X = (un) substituted C12-26
     dihydrocarbyl; counterion definitions not presented], having
     antimalarial and (veterinarian) antibabesiasis (e.g.,
     anti-piroplasmosis) activities, are prepd. and a I-contg. formulation
     claimed. Thus, 1,21-dibromoheneicosane was reacted with MeNEt2, producing
     N, N'-dimethyl-N, N, N', N'-tetraethyl-1, 21-heneicosanediammonium dibromide
     (m.p. 205), which demonstrated an in-vitro IC50 assay of 0.000003 .mu.M
     against Babesia bovis and Babesia canis and a therapeutic index of 12.
    ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2003 ACS
L51
     1997:638456 HCAPLUS
AN
     127:287699
DN
     Antimalarial Activity of Molecules Interfering with
TI
     Plasmodium falciparum Phospholipid Metabolism.
     Structure-Activity Relationship Analysis
     Calas, Michele; Cordina, Gerard; Bompart, Jacques; Bari, Mohamed
ΑU
     Ben; Jei, Taieb; Ancelin, Marie L.; Vial, Henri
```

- Laboratoire des Aminoacides Peptides et Proteines, ESA CNRS 5075, CS
- Montpellier, Fr. Journal of Medicinal Chemistry (1997), 40(22), 3557-3566 SO
- American Chemical Society PB

CODEN: JMCMAR; ISSN: 0022-2623

- Journal DΤ
- English LA
- A series of 80 compds., primary, secondary, and tertiary amines and AΒ quaternary ammonium and bisammonium salts, most of them synthesized as potential choline or ethanolamine analogs, were tested against the in vitro growth of Plasmodium falciparum, the human malaria parasite. They were active over the 10-3-10-8 M concn. range. A structure-activity relationship study was carried out using autocorrelation vectors as structural descriptors, and multidimensional anal. Principal component anal., ascending hierarchical classification, and stepwise discriminant anal. showed that both the size and shape of the mol. were essential for antimalarial potency, making the lipophilicity and electronegativity distribution in the mol. space essential. Using the autocorrelogram describing the mol. shape and the electronegativity distribution on the mol. graph, 98% of the mols. were correctly classified either as poorly active or active with only three explanatory variables. The most active compds. were quaternary ammoniums salts whose nitrogen atom had only one long lipophilic chain of 11 or 12 methylene groups or the bisammoniums whose polar heads were linked by linear alkyl chains of 10 to 12 carbon atoms. The hydroxyethyl group of choline was not very beneficial, whereas the charge and substitutions of nitrogen (aimed at increasing lipophilicity) were essential for optimal interactions. A crude topog. model of the

ligand (choline) binding site was thus drawn up.

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ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2003 ACS
T.51
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1986:403415 HCAPLUS AN´

DN 105:3415

Quaternary ammonium compounds efficiently inhibit TIPlasmodium falciparum growth in vitro by impairment of choline transport

Ancelin, Marie L.; Vial, Henri J. ΑU

- Cent. Natl. Rech. Sci., Inst. Natl. Sante Rech. Med., Montpellier, 34100, CS
- Antimicrobial Agents and Chemotherapy (1986), 29(5), 814-20 SO CODEN: AMACCQ; ISSN: 0066-4804
- DT Journal
- LA English
- Hemicholinium 3, decamethonium, and decyltrimethylammonium previously were AB demonstrated to be efficient inhibitors of P. falciparum, with 50% inhibitory concns. of 4 .times. 10-6, 10-6, and 7 .times. 10-7M, resp. Lengthening of the alkyl chain of decyltrimethylammonium by successive addns. of 2 C atoms up to hexadecyltrimethylammonium resulted in a very low 50% inhibitory concn. of 5 .times. 10-7 M for dodecyltrimethylammonium. Hemicholinium 3 and decamethonium exerted their antiplasmodial activity regardless of the developmental stage of the parasite, whereas decyltrimethylammonium was particularly lethal for the mature forms. After infected erythrocytes with radioactive choline were supplied, the detn. of the water-sol. choline-contg. compds. as well as the assay of choline kinase activity showed that the specific inhibition of phosphatidylcholine biosynthesis is related to the impairment of choline entry into erythrocytes. Thus, the impairment of the transport of choline, a natural polar head group of phospholipids, appears to be lethal for P. falciparum in vitro and could be a reasonable approach for a new malaria chemotherapy.

=> d his

L7

L9

L12

L15

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E FR99-9471/AP, PRN

L11 S E3, E4

E WO2000-FR2122/AP, PRN

L2 1 S E3, E4

L3 1 S L1, L2 SEL RN

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L474 S E1-E74

4 S L4 AND CLH

L5 2 S L5 NOT C6/ES L6

3 S L5 NOT C12H17NO2

1 S L7 NOT L6 L8

70 S L4 NOT L5

25 S L9 AND 1 12 DODECANE? L10

10 S L10 AND C6/ES L11

8 S L11 NOT NCSC2/ES

6 S L12 AND 1/NC

L13 4 S L11 NOT L13 L14

2 S L14 NOT BR/ELS

L16 15 S L10 NOT L11-L15

L17 9 S L16 NOT NCSC2/ES

45 S L9 NOT L10-L17 L18

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119
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L23
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             7 S L23 AND NCSC2/ES
             28 S L7, L8, L13, L15, L17, L21
L25
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L26
             39 S L4 NOT L24-L26
L27
L28
             8 S L27 AND NCSC2/ES
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L29
L30
             15 S L24, L28
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L32
L33
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              1 S L32, L33
L34
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L35
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             85 S E3-E8
L36
                E CALAS M/AU
             31 S E3-E5, E8
L37
                E ANCELIN M/AU
L38
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                E BOURGUIGNON J/AU
            204 S E3, E5, E10, E12
L39
               E VIDAL V/AU
             34 S E3-E9, E14, E15
L40
               E RUBI E/AU
             13 S E3, E5
L41
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              E VIDAL SAILHANT V/AU
L44
              1 S E4
             1 S E2
L45
              E SAILHAN/AU
             3 S E4,E5
L46
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L47
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             7 S L48 AND (?MALAR? OR ?PLASMOD? OR ?FALCIPAR? OR ?PARASIT? OR ?
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              6 S L49 NOT L50
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L52
            255 S E1-E255
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FILE 'HCAPLUS' ENTERED AT 16:57:54 ON 03 FEB 2003

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY 0.21

SESSION 0.21

FULL ESTIMATED COST

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TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

Uploading 486.str

L1 STRUCTURE UPLOADED

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STR

Structure attributes must be viewed using STN Express query preparation.

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100.0% PROCESSED

3 ITERATIONS

0 ANSWERS

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FULL FILE PROJECTIONS: ONLINE **COMPLETE**

PROJECTED ITERATIONS: 8ATCH **COMPLETE**
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PROJECTED ANSWERS: 0 TO 0

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L2

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=> d 13 15-19
     ANSWER 15 OF 19 REGISTRY COPYRIGHT 2003 ACS
L3
RN
     321915-54-2 REGISTRY
     Formamide, N,N'-1,12-dodecanediylbis[N-[4-methoxy-1-methyl-2-
CN
     (propyldithio) -1-butenyl] - (9CI) (CA INDEX NAME)
FS
     3D CONCORD
MF
     C32 H60 N2 O4 S4
SR
     CA
     STN Files: CA, CAPLUS
LC
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                             OHC Me S-SPr-n
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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
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               1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
     ANSWER 16 OF 19 REGISTRY COPYRIGHT 2003 ACS
L3
     321915-53-1 REGISTRY
RN
     Formamide, N,N'-1,12-dodecanediylbis[N-[4-hydroxy-2-[(2-
CN
     hydroxyethyl)dithio]-1-methyl-1-butenyl]- (9CI) (CA INDEX NAME)
FS
     3D CONCORD
MF
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     CA
LC
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                               OHC Me S-S-CH2-CH2-OH
HO-CH_2-CH_2-S-S Me CHO
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L3
     ANSWER 17 OF 19 REGISTRY COPYRIGHT 2003 ACS
     321915-52-0 REGISTRY
RN
CN
     Formamide, N, N'-1, 12-dodecanediylbis [N-[4-hydroxy-1-methyl-2-
     [(phenylmethyl)dithio]-1-butenyl]- (9CI) (CA INDEX NAME)
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MF
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SR
     CA
LC
     STN Files: CA, CAPLUS
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HO-CH_2-CH_2-C-C-C-N-(CH_2)_{12}-N-C-C-CH_2-CH_2-OH
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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 18 OF 19 REGISTRY COPYRIGHT 2003 ACS
- RN 321915-51-9 REGISTRY
- CN Formamide, N,N'-1,12-dodecanediylbis[N-[4-hydroxy-1-methyl-2-
 - (propyldithio) -1-butenyl] (9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C30 H56 N2 O4 S4
- SR CA
- LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 19 OF 19 REGISTRY COPYRIGHT 2003 ACS
- RN 321915-50-8 REGISTRY
- CN Formamide, N, N'-1, 12-dodecanediylbis[N-[4-hydroxy-1-methyl-2-[[(tetrahydro-
- 2-furanyl)methyl]dithio]-1-butenyl]- (9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C34 H60 N2 O6 S4
- SR CA
- LC STN Files: CA, CAPLUS

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- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> d l3 1-14

- L3 ANSWER 1 OF 19 REGISTRY COPYRIGHT 2003 ACS
- RN 321915-93-9 REGISTRY
- CN Formamide, N,N'-1,12-dodecanediylbis[N-[4-(benzoyloxy)-1-methyl-2-(propyldithio)-1-butenyl]- (9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C44 H64 N2 O6 S4
- SR CA
- LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- ANSWER 2 OF 19 REGISTRY COPYRIGHT 2003 ACS L3
- RN 321915-92-8 REGISTRY
- Formamide, N,N'-1,12-dodecanediylbis[N-[2-[[2-(diethylamino)ethyl]dithio]-CN4-methoxy-1-methyl-1-butenyl]- (9CI) (CA INDEX NAME)
- 3D CONCORD FS
- C38 H74 N4 O4 S4 MF
- SR CA
- STN Files: CA, CAPLUS LC

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- ANSWER 3 OF 19 REGISTRY COPYRIGHT 2003 ACS L3
- RN321915-85-9 REGISTRY
- Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-CN dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1ethenediyl]]] ester, (2R,3R)-2,3-dihydroxybutanedioate (1:2) (9CI) (CA
 - INDEX NAME)
- FS STEREOSEARCH
- MF C50 H74 N4 O8 S2 . 2 C4 H6 O6
- SR
- LC STN Files: CA, CAPLUS
 - CM 1
 - CRN 321915-62-2
 - CMF C50 H74 N4 O8 S2

PAGE 1-B

CM 2

CRN 87-69-4

C4 H6 O6 CMF

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1962 TO DATE) 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 4 OF 19 REGISTRY COPYRIGHT 2003 ACS L3

321915-84-8 REGISTRY

RN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-CNdodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1ethenediyl]]] ester, ethanedioate (1:2) (9CI) (CA INDEX NAME)

C50 H74 N4 O8 S2 . 2 C2 H2 O4MF

SR CA

LC STN Files: CA, CAPLUS

> CM1

321915-62-2 CRN CMF C50 H74 N4 O8 S2

PAGE 1-A

PAGE 1-B

CM2

CRN 144-62-7 CMF C2 H2 O4

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 5 OF 19 REGISTRY COPYRIGHT 2003 ACS

RN321915-64-4 REGISTRY

CN Benzenecarbothioic acid, S,S'-[1,16-hexadecanediylbis[(formylimino)[1-(2methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

MF C44 H64 N2 O6 S2

SR

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 6 OF 19 REGISTRY COPYRIGHT 2003 ACS

RN 321915-63-3 REGISTRY

CN Benzoic acid, 4,4'-[5,18-diformyl-3,20-bis(2-methoxyethyl)-4,19-dimethyl-1,22-dioxo-2,21-dithia-5,18-diazadocosa-3,19-diene-1,22-diyl]bis-, dimethyl ester (9CI) (CA INDEX NAME)

MF C44 H60 N2 O10 S2

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 7 OF 19 REGISTRY COPYRIGHT 2003 ACS

RN 321915-62-2 REGISTRY

CN Benzenecarbothioic acid, 4-(4-morpholinylmethyl)-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

MF C50 H74 N4 O8 S2

CI COM

SR CA

LC STN Files: CA, CAPLUS

PAGE 1-B

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 8 OF 19 REGISTRY COPYRIGHT 2003 ACS

RN 321915-61-1 REGISTRY

CN Benzenecarbothioic acid, 4-[(diethylamino)methyl]-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester, dihydrochloride (9CI) (CA INDEX NAME)

MF C50 H78 N4 O6 S2 . 2 C1 H

SR CA

LC STN Files: CA, CAPLUS

•2 HCl

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 9 OF 19 REGISTRY COPYRIGHT 2003 ACS
- RN 321915-60-0 REGISTRY
- CN Benzenecarbothioic acid, 4-[2-(4-morpholinyl)ethoxy]-,

S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-

ethenediyl]]] ester (9CI) (CA INDEX NAME)

MF C52 H78 N4 O10 S2

SR CF

LC STN Files: CA, CAPLUS

PAGE 1-B

- CH₂- OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 10 OF 19 REGISTRY COPYRIGHT 2003 ACS

RN 321915-59-7 REGISTRY

CN Benzenecarbothioic acid, 4-methoxy-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

MF C42 H60 N2 O8 S2

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 11 OF 19 REGISTRY COPYRIGHT 2003 ACS
- RN 321915-58-6 REGISTRY
- CN Benzenecarbothioic acid, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-

methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)

- MF C40 H56 N2 O6 S2
- SR CA
- LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 12 OF 19 REGISTRY COPYRIGHT 2003 ACS
- RN 321915-57-5 REGISTRY
- CN Propanethioic acid, 2,2-dimethyl-, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
- MF C36 H64 N2 O6 S2
- SR CA
- LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 13 OF 19 REGISTRY COPYRIGHT 2003 ACS
- RN 321915-56-4 REGISTRY
- CN Ethanethioic acid, S,S'-[1,12-dodecanediylbis[(formylimino)[1-(2-methoxyethyl)-2-methyl-2,1-ethenediyl]]] ester (9CI) (CA INDEX NAME)
- MF C30 H52 N2 O6 S2
- SR CA
- LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 14 OF 19 REGISTRY COPYRIGHT 2003 ACS
- RN 321915-55-3 REGISTRY
- CN Formamide, N,N'-1,12-dodecanediylbis[N-[1-methyl-2-(propyldithio)ethenyl]-(9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C26 H48 N2 O2 S4
- SR CA
- LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

ENTRY SESSION 180.47 180.68

FILE 'CAPLUS' ENTERED AT 16:21:51 ON 05 FEB 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 5 Feb 2003 VOL 138 ISS 6 FILE LAST UPDATED: 4 Feb 2003 (20030204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s 13
L4 1 L3
```

=> d

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

AN 2001:63952 CAPLUS

DN 134:131521

TI Preparation of neutral prodrugs of bisquaternaryammonium parasiticides

IN Vial, Henri; Calas, Michele; Ancelin, Marie-Laure; Bourguignon, Jean-Jacques; Vidal, Valerie; Rubi, Eric

PA Centre National de la Recherche Scientifique (C.N.R.S.), Fr.

SO PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DT Patent

LA French

| FAN | CNT | 1 | | | | | | | | | | | | | | | | |
|------|-----|--------|------|-----|-----|-----|------|------|-----|-----|------|------|------|------|------|------|-----|-----|
| 1121 | | CENT : | NO. | | KI | ND | DATE | | | A. | PPLI | CATI | ON N | o. : | DATE | | | |
| | | | | | | | | | | - | | | | | | | | |
| ΡI | WO | 2001 | 0057 | 42 | Α | 1 | 2001 | 0125 | | W | 20 | 00-F | R212 | 2 | 2000 | 0721 | | |
| | | W: | ΑE, | AG, | AL, | AM, | ΑT, | AU, | ΑZ, | BA, | BB, | BG, | BR, | BY, | ΒZ, | CA, | CH, | CN, |
| | | | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EE, | ES, | FI, | GB, | GD, | GE, | GH, | GM, | HR, |
| | | | HU, | ID, | IL, | IN, | ıs, | JP, | KE, | KG, | ΚP, | KR, | KZ, | LC, | LK, | LR, | LS, | LT, |
| | | | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NO, | NZ, | ΡL, | PT, | RO, | RU, |
| | | | SD, | SE, | SG, | SI, | SK, | SL, | ТJ, | TM, | TR, | TT, | TZ, | UA, | UG, | US, | UΖ, | VN, |
| | | | YU, | ZA, | ZW, | AM, | ΑZ, | BY, | KG, | ΚZ, | MD, | RU, | ТJ, | TM | | | | |
| | | RW: | GH, | GM, | KE, | LS, | MW, | MZ, | SD, | SL, | SZ, | TZ, | UG, | ZW, | ΑT, | ΒE, | CH, | CY, |
| | | | DE, | DK, | ES, | FI, | FR, | GB, | GR, | ΙE, | IT, | LU, | MC, | NL, | PT, | SE, | BF, | ВJ, |
| | | | CF, | CG, | CI, | CM, | GΑ, | GN, | GW, | ML, | MR, | ΝE, | SN, | TD, | TG | | | |

19990721 FR 2796642 A1 20010126 FR 1999-9471 B1 20011019 FR 2796642 EP 2000-958598 20000721 A1 20020417 EP 1196371 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO BR 2000-12601 20000721 BR 2000012601 A 20020521 19990721 PRAI FR 1999-9471 Α WO 2000-FR2122 W 20000721 MARPAT 134:131521 OS THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 8

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 1.43 182.11

FULL ESTIMATED COST

FILE 'CAOLD' ENTERED AT 16:22:26 ON 05 FEB 2003
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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s 13

0 L3

FILE 'HOME' ENTERED AT 16:27:26 ON 05 FEB 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 16:27:36 ON 05 FEB 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5 DICTIONARY FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

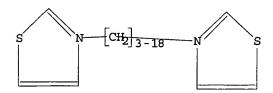
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 486.str

L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:27:54 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 143 TO ITERATE

100.0% PROCESSED 143 ITERATIONS

5 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** PROJECTED ITERATIONS: 2143 TO 3577 PROJECTED ANSWERS: 5 TO 234

=> d 12 5

L2 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2003 ACS

RN 47358-00-9 REGISTRY

CN Benzothiazolium, 3,3'-(1,6-hexanediyl)bis- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H22 N2 S2

CI COM

=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

2.88 3.09

FULL ESTIMATED COST

FILE 'STNGUIDE' ENTERED AT 16:29:10 ON 05 FEB 2003
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 31, 2003 (20030131/UP).

Uploading

oproading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY 0.06 SESSION 3.15

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 16:29:50 ON 05 FEB 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5 DICTIONARY FILE UPDATES: 4 FEB 2003 HIGHEST RN 485752-98-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

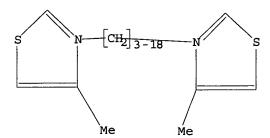
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

Uploading 486.str

L3 STRUCTURE UPLOADED

=> d L3 HAS NO ANSWERS STR

L3



Structure attributes must be viewed using STN Express query preparation.

=> s 13 SAMPLE SEARCH INITIATED 16:30:04 FILE 'REGISTRY' 9 TO ITERATE SAMPLE SCREEN SEARCH COMPLETED -

100.0% PROCESSED 9 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

PROJECTED ITERATIONS: 9 TO 360 PROJECTED ANSWERS: 1 TO 80

1 SEA SSS SAM L3 L4

=> d

ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS L4

RN

321915-73-5 REGISTRY
Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-methoxyethyl)-4-methyl-, dibromide (9CI) (CA INDEX NAME) CN

C26 H46 N2 O2 S2 . 2 Br MF

SR CA

LC STN Files: CA, CAPLUS

$$CH_2-CH_2-OMe$$
 N_+
 Me
 $(CH_2)_{12}$
 N_+
 Me
 S
 CH_2-CH_2-OMe

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> s 13 ful

FULL SEARCH INITIATED 16:30:29 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 266 TO ITERATE

100.0% PROCESSED 266 ITERATIONS 22 ANSWERS

SEARCH TIME: 00.00.01

22 SEA SSS FUL L3 L5

=> d 15 1-22

L5 ANSWER 1 OF 22 REGISTRY COPYRIGHT 2003 ACS

477526-11-7 REGISTRY RN

INDEX NAME NOT YET ASSIGNED CN

C26 H32 N4 S2 . 2 Br MF

SR Chemical Library

PhNH
$$N + Me$$

(CH₂) 6

PhNH $N + Me$

2 Br -

ANSWER 2 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

321915-75-7 REGISTRY RN

Thiazolium, 3,3'-(1,16-hexadecanediyl)bis[5-(2-methoxyethyl)-4-methyl-, diodide (9CI) (CA INDEX NAME)
C30 H54 N2 O2 S2 . 2 I CN

MF

SR

LC STN Files: CA, CAPLUS

$$S$$
 N_{+}
 Me
 $(CH_{2})_{16}$
 N_{+}
 Me
 S
 $CH_{2}-CH_{2}-OMe$
 S

2 I-

1 REFERENCES IN FILE CA (1962 TO DATE) 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 3 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

321915-74-6 REGISTRY RN

Thiazolium, 3,3'-(1,12-dodecanediyl)bis[4-methyl-, diiodide (9CI) (CA CNINDEX NAME)

MF C20 H34 N2 S2 . 2 I

SR

STN Files: CA, CAPLUS LC

2 I-

1 REFERENCES IN FILE CA (1962 TO DATE) 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 4 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

321915-73-5 REGISTRY RN

Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-methoxyethyl)-4-methyl-, dibromide (9CI) (CA INDEX NAME)
C26 H46 N2 O2 S2 . 2 Br CN

MF

SR

STN Files: CA, CAPLUS LC

$$S$$
 N_{+}
 CH_{2}
 CH_{2}
 OMe
 N_{+}
 CH_{2}
 OMe
 N_{+}
 OMe
 N_{+}
 OMe
 N_{+}
 OMe
 OMe

1 REFERENCES IN FILE CA (1962 TO DATE) 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 5 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

321915-72-4 REGISTRY RN

Thiazolium, 3,3'-(1,12-dodecanediyl)bis[5-(2-hydroxyethyl)-4-methyl-, CN

dibromide (9CI) (CA INDEX NAME) C24 H42 N2 O2 S2 . 2 Br

MF

SR CA

LC STN Files: CA, CAPLUS

2 Br-

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 6 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

146891-88-5 REGISTRY RN

Thiazolium, 3,3'-(1,8-octanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA CNINDEX NAME)

MFC18 H30 N2 S2 . 2 Br

SR

LC STN Files: CA, CAPLUS

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 7 OF 22 REGISTRY COPYRIGHT 2003 ACS

RN 146891-87-4 REGISTRY

CN Thiazolium, 3,3'-(1,7-heptanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)

MF C17 H28 N2 S2 . 2 Br

SR CA

LC STN Files: CA, CAPLUS

2 Br -

- 2 REFERENCES IN FILE CA (1962 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L5 ANSWER 8 OF 22 REGISTRY COPYRIGHT 2003 ACS
- RN 146891-86-3 REGISTRY
- CN Thiazolium, 3,3'-(1,6-hexanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)
- MF C16 H26 N2 S2 . 2 Br
- SR CA
- LC STN Files: CA, CAPLUS

3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 9 OF 22 REGISTRY COPYRIGHT 2003 ACS

RN 146891-85-2 REGISTRY

CN Thiazolium, 3,3'-(1,5-pentanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)

MF C15 H24 N2 S2 . 2 Br

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

2 Br -

- 2 REFERENCES IN FILE CA (1962 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 10 OF 22 REGISTRY COPYRIGHT 2003 ACS

RN 146891-84-1 REGISTRY

CN Thiazolium, 3,3'-(1,4-butanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)

MF C14 H22 N2 S2 . 2 Br

SR CA

LC STN Files: CA, CAPLUS

2 Br -

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 11 OF 22 REGISTRY COPYRIGHT 2003 ACS

RN 146891-83-0 REGISTRY

CN Thiazolium, 3,3'-(1,3-propanediyl)bis[4,5-dimethyl-, dibromide (9CI) (CA INDEX NAME)

MF C13 H20 N2 S2 . 2 Br

SR CA

LC STN Files: CA, CAPLUS

2 Br-

2 REFERENCES IN FILE CA (1962 TO DATE)

2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 12 OF 22 REGISTRY COPYRIGHT 2003 ACS

RN 105420-27-7 REGISTRY

CN Thiazolium, 3,3'-(1,8-octanediyl)bis[4-methyl-, dibromide (9CI) (CA INDEX NAME)

MF C16 H26 N2 S2 . 2 Br

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1962 TO DATE) 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 13 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

105420-26-6 REGISTRY RN

Thiazolium, 3,3'-(1,6-hexanediyl)bis[4-methyl-, dibromide (9CI) (CA INDEX CNNAME)

MF C14 H22 N2 S2 . 2 Br

SR

LC STN Files: CA, CAPLUS

2 Br-

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- ANSWER 14 OF 22 REGISTRY COPYRIGHT 2003 ACS 105420-25-5 REGISTRY L5
- RN
- Thiazolium, 3,3'-(1,5-pentanediyl)bis[4-methyl-, dibromide (9CI) CNINDEX NAME)
- ΜF C13 H20 N2 S2 . 2 Br
- SR
- LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

1 REFERENCES IN FILE CA (1962 TO DATE) 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 15 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

105420-24-4 REGISTRY RN

Thiazolium, 3,3'-(1,3-propanediyl)bis[4-methyl-, dibromide (9CI) (CA CNINDEX NAME)

C11 H16 N2 S2 . 2 Br ΜF

SR

LC STN Files: CA, CAPLUS, CASREACT

2 Br -

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- ANSWER 16 OF 22 REGISTRY COPYRIGHT 2003 ACS L5
- RN
- 97745-74-9 REGISTRY Thiazolium, 3,3'-(1,4-butanediyl)bis[4-methyl-, dibromide (9CI) (CA INDEX CNNAME)
- MF C12 H18 N2 S2 . 2 Br
- SR
- STN Files: CA, CAPLUS, CASREACT LC

3 REFERENCES IN FILE CA (1962 TO DATE) 3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 17 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

87051-17-0 REGISTRY RN

Thiazolium, 3,3'-(1,6-hexanediyl)bis[4-methyl-, dichloride (9CI) (CA CNINDEX NAME)

C14 H22 N2 S2 . 2 Cl MF

●2 Cl-

ANSWER 18 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

RN

76800-93-6 REGISTRY
Thiazolium, 3,3'-(1,3-propanediyl)bis[5-(2-chloroethyl)-4-methyl-, CNdiiodide (9CI) (CA INDEX NAME)

C15 H22 Cl2 N2 S2 . 2 I MF

LCSTN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

$$S \longrightarrow Me$$
 N_{+}
 $CH_{2}-CH_{2}C1$
 Me
 CH_{2}
 N_{+}
 $CH_{2}-CH_{2}C1$
 N_{+}
 $CH_{2}-CH_{2}C1$

2 I-

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 19 OF 22 REGISTRY COPYRIGHT 2003 ACS

RN 54642-19-2 REGISTRY

CN Thiazolium, 3,3'-(1,5-pentanediyl)bis[2,4-dimethyl-, dibromide (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 3,3'-Pentamethylenebis(2,4-dimethylthiazolium bromide)

MF C15 H24 N2 S2 . 2 Br

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Me
$$N_+$$
 Me $(CH_2)_5$ N_+ Me N_+ Me

2 Br-

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L5 ANSWER 20 OF 22 REGISTRY COPYRIGHT 2003 ACS

RN 54642-18-1 REGISTRY

CN Thiazolium, 3,3'-(1,4-butanediyl)bis[2,4-dimethyl-, diiodide (9CI) (CA INDEX NAME)

MF C14 H22 N2 S2 . 2 I

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Me
$$N_+$$
 Me $(CH_2)_4$ Me N_+ Me

2 I-

1 REFERENCES IN FILE CA (1962 TO DATE) 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 21 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

54642-17-0 REGISTRY RN

Thiazolium, 3,3'-(1,3-propanediyl)bis[2,4-dimethyl-, diperchlorate (9CI) CN (CA INDEX NAME)

OTHER NAMES:

3-3'-Trimethylenebis (2,4-dimethylthiazolium perchlorate CN

 $\tt C13\ H20\ N2\ S2$. 2 Cl $\tt O4$ MF

STN Files: CA, CAPLUS LC

> CM 1

CRN 54642-16-9 CMF C13 H20 N2 S2

CM

CRN 14797-73-0 CMF Cl O4

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 22 OF 22 REGISTRY COPYRIGHT 2003 ACS L5

RN

54642-16-9 REGISTRY Thiazolium, 3,3'-(1,3-propanediyl)bis[2,4-dimethyl- (9CI) (CA INDEX NAME) CN

FS 3D CONCORD

MFC13 H20 N2 S2

Me
$$N_{+}$$
 Me $(CH_{2})_{3}$ N_{+} Me

=> file caplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 187.19 190.34

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FILE COVERS 1907 - 5 Feb 2003 VOL 138 ISS 6 FILE LAST UPDATED: 4 Feb 2003 (20030204/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L6 9 L5
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=> d 16 1-9

L6 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2003 ACS

AN 2001:63952 CAPLUS

DN 134:131521

TI Preparation of neutral prodrugs of bisquaternaryammonium parasiticides

IN Vial, Henri; Calas, Michele; Ancelin, Marie-Laure; Bourguignon,

Jean-Jacques; Vidal, Valerie; Rubi, Eric

PA Centre National de la Recherche Scientifique (C.N.R.S.), Fr.

SO PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DT Patent LA French

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2001005742 A1 20010125 WO 2000-FR2122 20000721

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,

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SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
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             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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     A kinetic study by NMR of the benzoin condensation catalyzed by thiazolium
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     salts in mild basic conditions: a second order process in both aldehyde
     and pre-catalyst
     Lopez-Calahorra, Francisco; Rubires, Raimon
ΑU
     Department Quimica Organica, Universitat Barcelona, Barcelona, E-08028,
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     Use of 3,3'-polymethylene-bridged thiazolium salts plus bases as catalysts
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     a new mechanism in aprotic conditions
     Lopez-Celahorra, Francisco; Castells, Josep; Domingo, Laura; Marti, Josep;
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     Bofill, Josep M.
     Dep. Quimica Organica, Univ. Barcelona, Barcelona, 08028, Spain
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ΑU
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